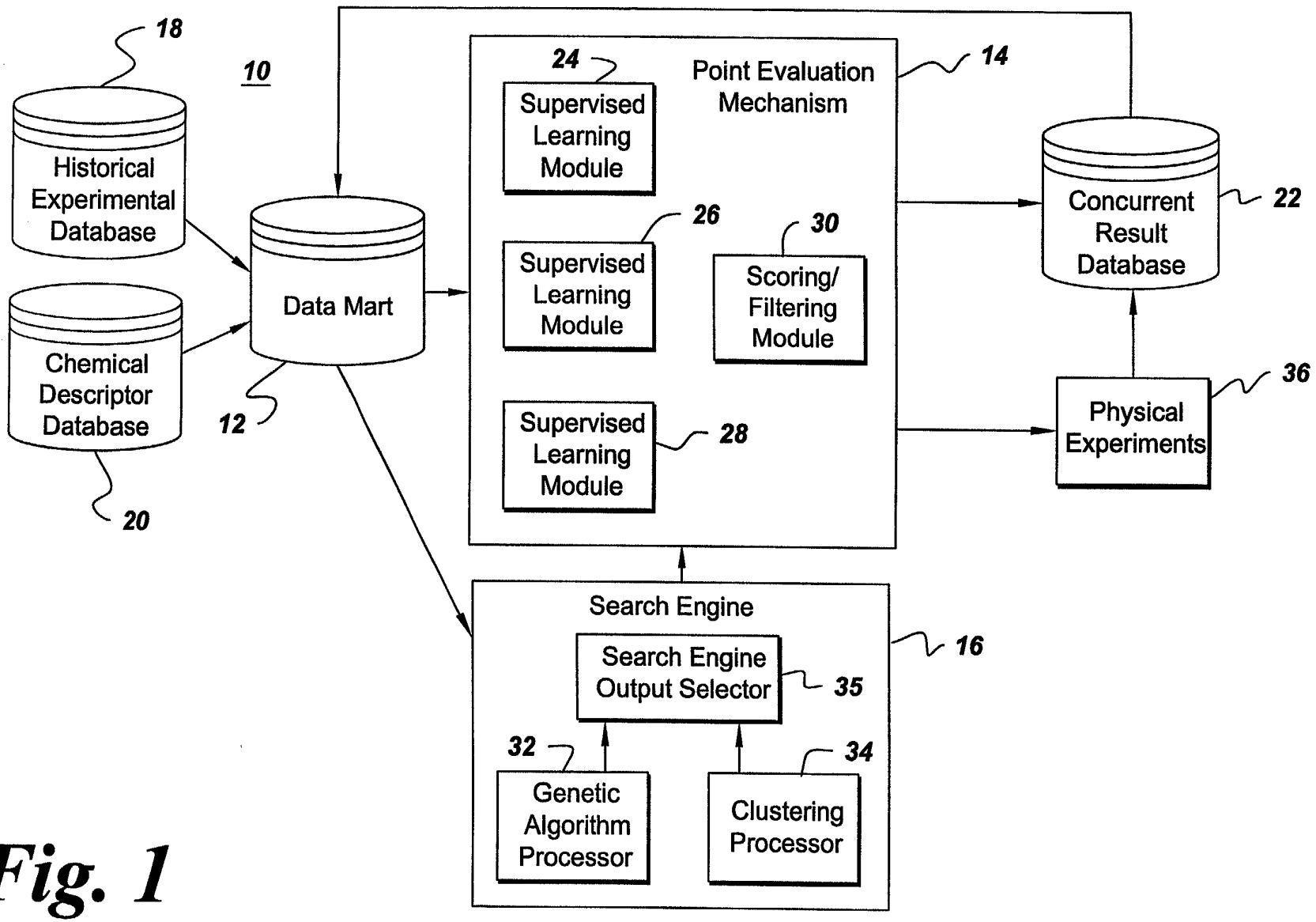
18
10
Historical Experimental Database
Chemical Descriptor Database
20
Data Mart
12
24
Supervised Learning Module
Point Evaluation Mechanism
14
26
Supervised Learning Module
30
Scoring/ Filtering Module
Supervised Learning Module
28
Concurrent Result Database
22
Physical Experiments
36
Search Engine
16
Search Engine Output Selector
35
32
Genetic Algorithm Processor
34
Clustering Processor

Fig. 1

TO6250 SHEETS260

40

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Bi	Ca	Cd	Ce	Co	Cr	Cs	Cu	Eu	Fe	Gd	In	Ir	La	Mn	Ni	ReO	Rh	Ru	TiO	Yb	Zn	Avg TON
0	0	0	1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1802
1	0	0	0	0	0	0	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	1711
1	0	0	0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1698
0	0	0	0	0	0	1	0	0	1	0	0	0	1	0	0	0	0	0	0	0	0	1671
1	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	0	0	0	0	0	1670
0	0	0	1	0	0	1	0	0	0	0	0	0	0	0	0	0	1	0	0	0	0	1645
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0	0	0	1	0	0	0	1	0	1	0	0	0	0	0	0	0	0	0	0	0	0	1506

Fig. 2

46

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Metal	Electro-negativity	Atomic Radius	Covalent Radius	Ionization Potential	Atomic Ionization Potential I	II	III	IV	Electron Affinity
Bi	1.67	1.7	1.46	7.29	7.29	16.16	25.56	45.3	0.95
Ca	1.04	1.97	1.74	6.11	6.11	11.9	50.908	67.1	0.18
Cd	1.46	1.54	1.48	9	8.99	16.91	37.48	NA	NA
Ce	1.06	1.81	1.65	5.53	5.47	10.85	20.2	36.72	NA
Co	1.7	1.3	NA	7.87	7.86	17.06	33.5	51.3	0.662
Cr	1.56	1.27	NA	6.76	6.76	16.5	30.96	49.1	0.666
Cs	0.86	2.67	2.25	3.89	3.89	25.1	NA	NA	0.47
Cu	1.75	1.28	1.38	7.73	7.726	20.29	36.83	55.2	1.235
Eu	1.01	2.04	1.85	5.68	5.67	11.25	24.9	NA	NA
Fe	1.64	0.68	0.72	7.9	7.87	16.18	30.65	54.8	0.151
Ga	1.82	1.4	1.26	6	6	20.51	30.71	64	0.3
In	1.49	1.66	144	5.79	5.78	18.87	28.03	54	0.3
Ir	1.55	1.36	NA	9	9.1	NA	NA	NA	1.565
La	1.08	1.86	1.69	5.61	5.57	11.06	19.1	NA	NA
Mn	1.6	1.26	NA	7.43	7.43	15.64	33.66	51.2	NA
Ni	1.75	1.24	NA	7.63	7.63	18.17	35.17	54.9	1.156
Pb	1.55	1.75	1.47	7.417	7.416	15.032	31.94	42.32	NA
Re	1.46	1.37	NA	7.87	7.9	NA	NA	NA	0.15
Rh	1.45	1.34	NA	7.46	7.46	18.08	31.06	NA	1.137
Ru	1.42	1.33	NA	7.37	7.37	16.76	28.47	NA	1.05
Sb	1.82	1.5	1.38	8.641	8.64	16.53	25.3	44.2	NA
Sn	1.72	1.5	1.41	7.344	7.34	14.63	30.5	40.7	NA
Ti	1.32	1.45	1.36	6.82	6.82	13.58	27.49	43.26	0.079
Yb	1.06	1.93	1.7	6.22	6.25	12.17	25	NA	0.5
Zn	1.66	1.38	1.31	9.39	9.394	17.964	39.722	59.4	NA
Zr	1.22	1.6	1.48	6.835	6.84	13.13	22.99	34.34	NA

Fig. 3

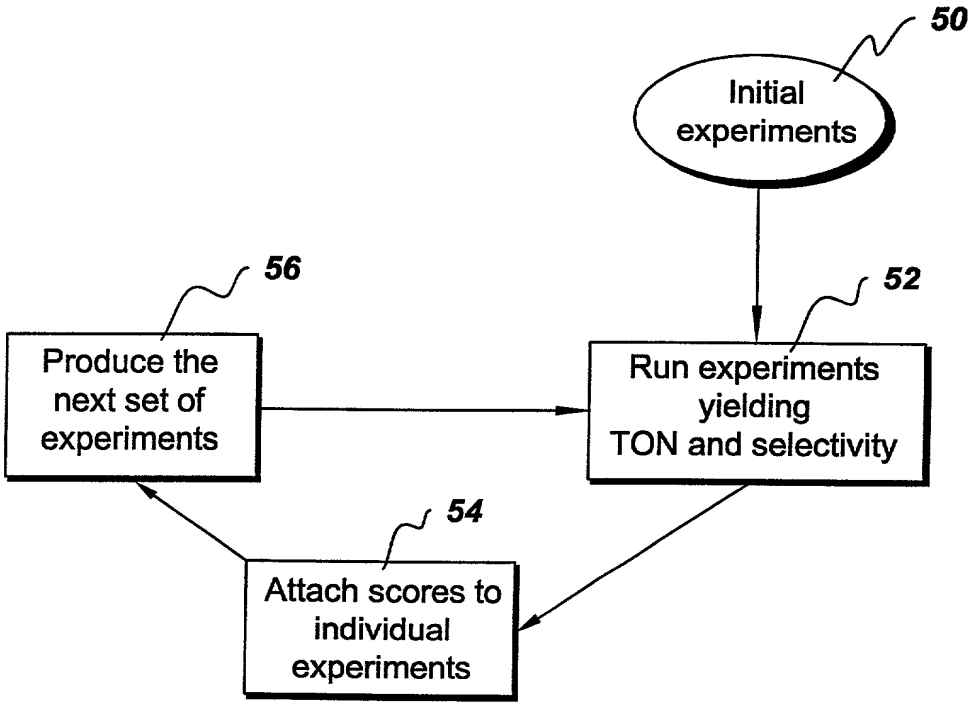
50
Initial experiments
52
Run experiments yielding TON and selectivity
54
Attach scores to individual experiments
56
Produce the next set of experiments

Fig. 4

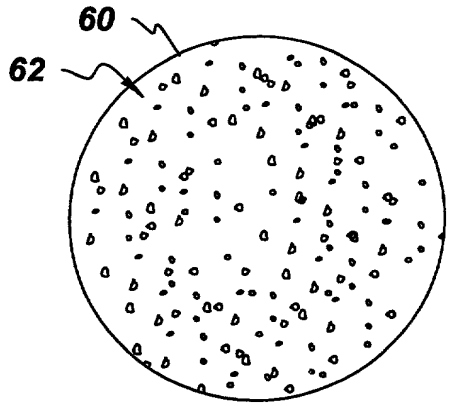
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Fig. 5

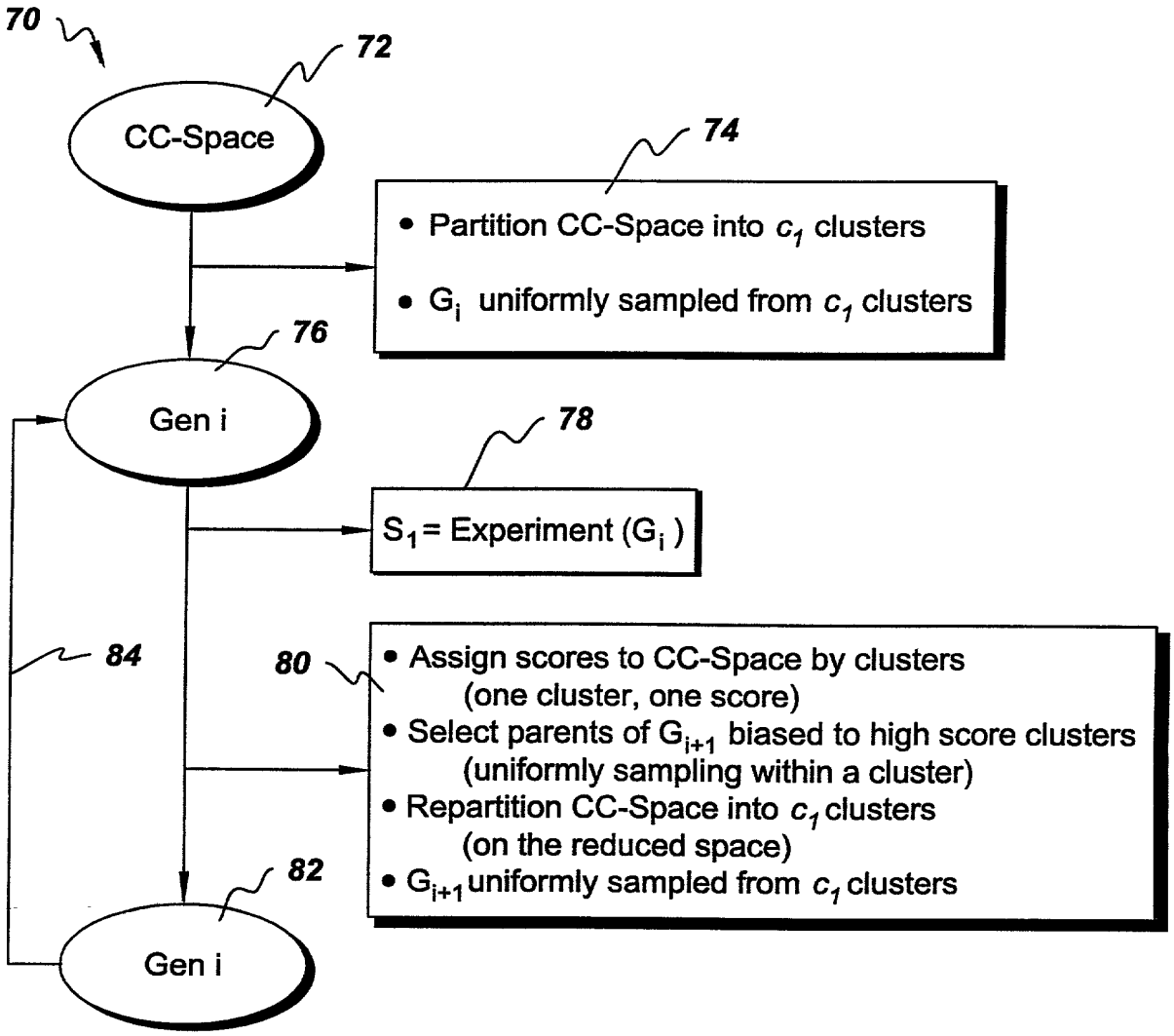
70
72
CC-Space
74
• Partition CC-Space into c_1 clusters
• G_i uniformly sampled from c_1 clusters
76
Gen i
78
S_1 = Experiment (G_i)
84
80
• Assign scores to CC-Space by clusters (one cluster, one score)
• Select parents of G_{i+1} biased to high score clusters (uniformly sampling within a cluster)
• Repartition CC-Space into c_1 clusters (on the reduced space)
• G_{i+1} uniformly sampled from c_1 clusters
82
Gen i

Fig. 6

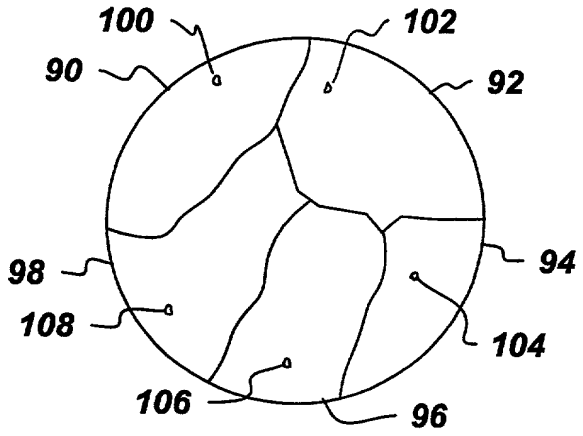

Fig. 7

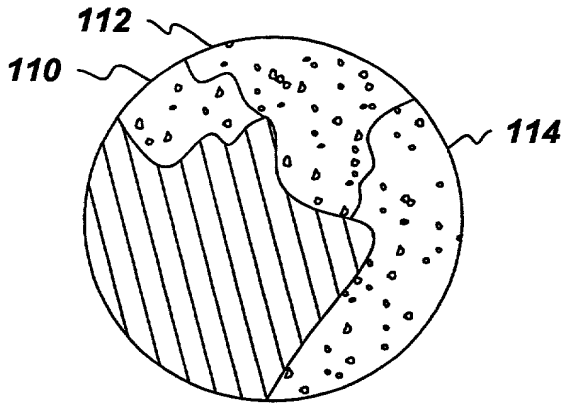

Fig. 8

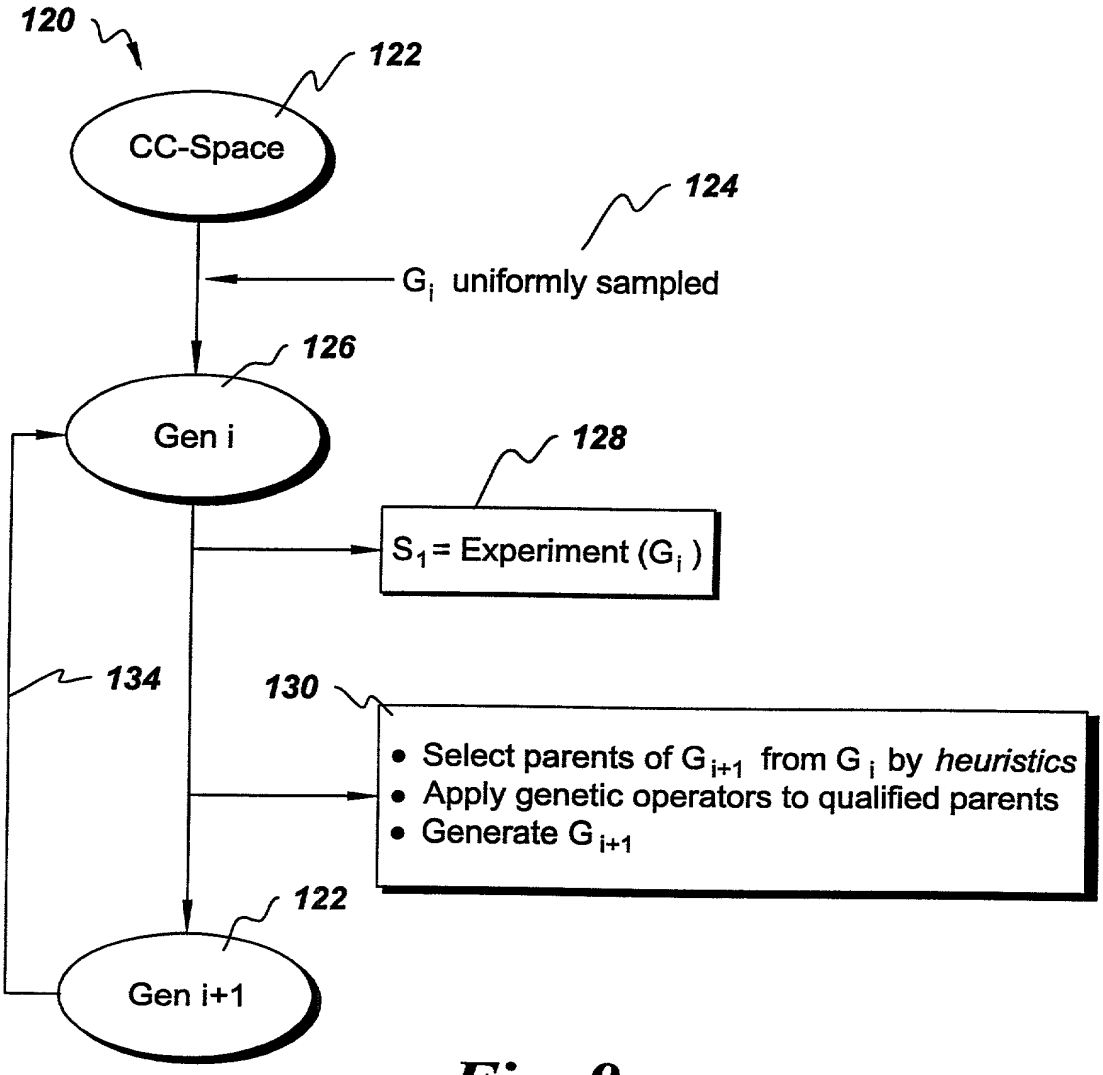

Fig. 9

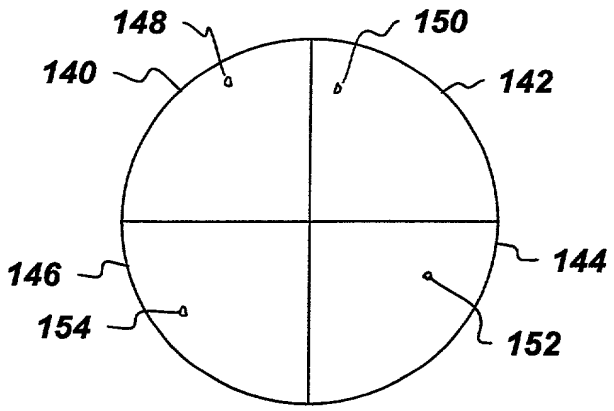
148
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Fig. 10

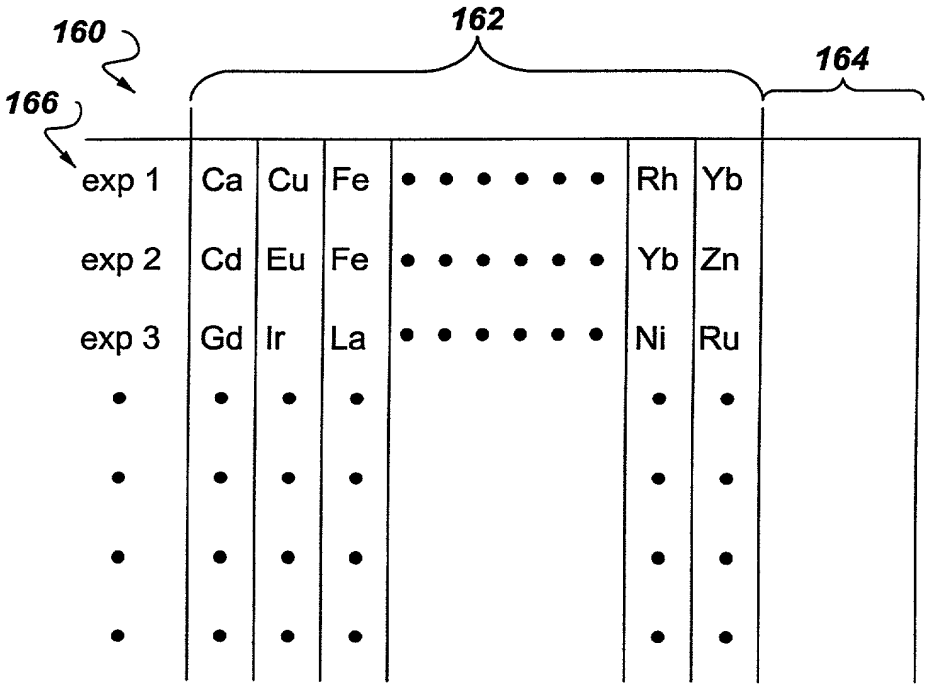
160
162
164
166
exp 1 Ca Cu Fe • • • • • • Rh Yb
exp 2 Cd Eu Fe • • • • • • Yb Zn
exp 3 Gd Ir La • • • • • • Ni Ru

Fig. 11

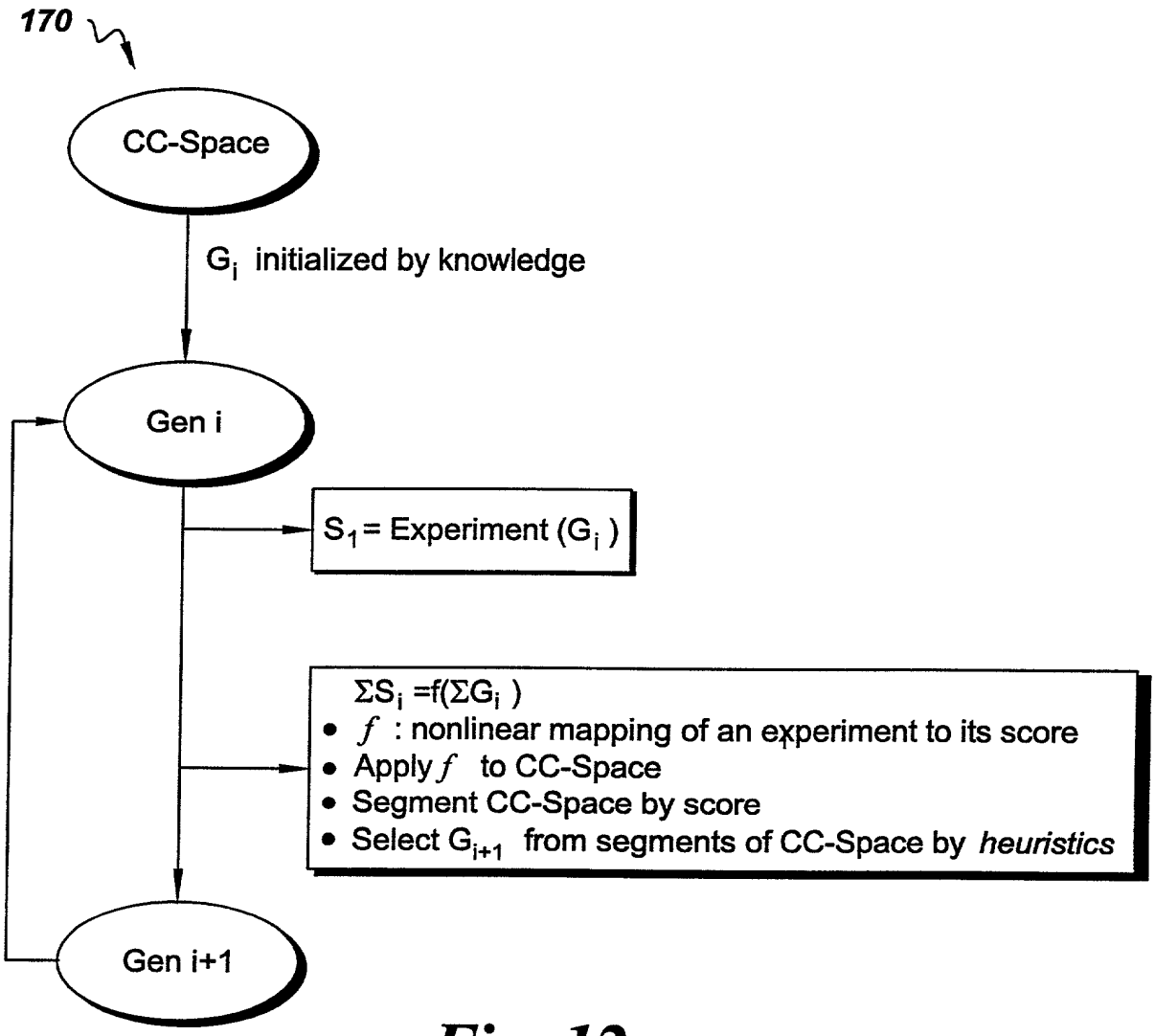
170
CC-Space
G_i initialized by knowledge
Gen i
S_1 = Experiment (G_i)
$\Sigma S_i = f(\Sigma G_i)$
• f : nonlinear mapping of an experiment to its score
• Apply f to CC-Space
• Segment CC-Space by score
• Select G_{i+1} from segments of CC-Space by *heuristics*
Gen i+1

Fig. 12